

UMAT Implementation of Coupled, Multilevel, Structural Deformation and Damage Analysis of General Hereditary Materials

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Abstract

Extensive research efforts have been made over the years on the phenomenological representations of constitutive material behavior in the inelastic analysis and life assessment of structures composed of advanced monolithic and composite (CMC, MMC, and PMC) materials. Recently, emphasis has been placed on concurrently addressing three important and related areas of constitutive and degradation modeling; i.e. (i) mathematical formulation, (ii) algorithmic developments for the updating (integrating) of external (e.g. stress) and internal state variable, as well as (iii) parameter estimation for the characterization of the specific model. This concurrent perspective has resulted in; i) the formulation of a fully-associative viscoelastoplastic model (GVIPS), (ii) development of an efficient implicit integration and its associative, symmetric, consistent tangent stiffness matrix algorithm for integration of the underlying rate flow/evolutionary equations, and iii) a robust, stand-alone, Constitutive Material Parameter Estimator (COMPARE) for automatically characterizing the various time-dependent, nonlinear, material models.

Furthermore, to provide a robust multi-scale framework for the deformation and life analysis of structures composed of composite materials, NASA Glenn has aggressively pursued the development of a sufficiently general, accurate, and efficient micromechanics approach known as the generalized method of cells (GMC). This work has resulted in the development of MAC/GMC, a stand-alone micromechanics analysis tool that can easily and accurately design/analyze multi-

phase (composite) materials subjected to complex histories. MAC/GMC admits generalized, physically based, deformation and damage models for each constituent and provides "closed-form" expressions for the macroscopic composite response in terms of the properties, size, shape, distribution, and response of the individual constituents or phases that comprise the material. Consequently, MAC/GMC can be incorporated directly into a structural finite element code like ABAQUS for cost-effective, micromechanics based, large-scale component design and analysis.

Our primary objective here is to report on these recent works conducted over the past decade, in the context of their incorporation into ABAQUS through the various user subroutines. Representative results will be shown to demonstrate the features of the developed schemes.

INTRODUCTION

The use of advanced composites (PMCs, MMCs, CMCs) provides potential benefits in the design of advanced engines because they can provide increased strength to density ratios in comparison to the current monolithic materials used at temperatures of interest. To fully realize the benefits offered by these materials, however, experimentally verified, computationally efficient design and life prediction methods must be developed for the advanced multiphased materials of interest in advanced engine and propulsion systems. Consequently, these analysis tools must admit physically based, hereditary deformation and life models and be compatible with the finite element method, in order to describe accurately the complex thermomechanical load histories typical in the aerospace structures of interest. Furthermore, in order to assist both the structural analyst and the material scientist in developing and utilizing these materials, these tools must encompass the various levels of scale for composite analysis, see Fig 1.

To respond to this difficult challenge, continuum based theoretical modeling of composite deformation and damage is being pursued through two parallel approaches at the National Aeronautics and Space Administration Glenn Research Center (NASA GRC). The distinguishing feature between the two approaches (see Fig. 1) is their relative starting point, wherein one begins at the microscale (constituent level) and the other at the macroscale (laminate, or composite level), each with unique needs in terms of experimental characterization and verification. The simultaneous pursuit of two parallel, yet not mutually exclusive, approaches is motivated by two key considerations. First, at this time in their respective developments it is not apparent that one

approach is superior to the other, relative to the primary goal of developing accurate, computationally efficient, and experimentally validated analysis tools. Second, it is clear that each approach has its realm of applicability with obvious strengths and weaknesses.

For example, the microscale approach (micromechanics) is thought to be most suited for applications involving fabrication and material development, where an accurate evaluation of the micro-stresses and -strains are critical. However, this detailed information often comes at great computational cost, which often renders the approach impractical and prohibitive for the design and analysis of structural components. In contrast, the macroscale approach (macromechanics) is clearly the more computationally efficient, thereby facilitating its use in large-scale component design and analysis. This efficiency, however, may come at the cost of accuracy in comparison to its more computationally intense micro counterpart; particularly when highly localized, non-uniform behavior (relative to the representative volume element (RVE)) dominates. Consequently, with these given considerations, both micro- and macro-based theoretical approaches continue to be pursued and refined in a parallel fashion at GRC with the ultimate goal being the development of a multiscale functional framework that is both computationally efficient and accurate for deformation and life analysis under general nonisothermal, multiaxial loadings.

This multiscale framework is depicted schematically in Fig. 2, wherein it is segmented into three interconnected disciplines, 1) characterization/validation, 2) structural analysis, and 3) detection techniques. Here we will confine our discussion to primarily the structural analysis segment; in particular, the deformation modeling, damage modeling, and micromechanics homogenization sub-segments which have been incorporated into ABAQUS through the various user subroutines.

DEFORMATION MODELING

An integral part of continuum based computational methodologies (be they microscale- or macroscale-based) is an accurate and computationally efficient constitutive model to describe the deformation behavior of the materials of interest. Extensive research efforts have been made over the years on the **phenomenological** representations of constitutive material behavior in the inelastic analysis of structures. From a more recent and comprehensive perspective (Saleeb et al., 2000), emphasis has been placed on concurrently addressing three important and related areas;

i.e., (i) **mathematical** formulation, (ii) **algorithmic** developments for the updating (integrating) of external (e.g., stress) and internal state variables, as well as (iii) **parameter estimation** for the characterization of the model. This concurrent perspective to constitutive modeling has enabled the overcoming of the two major obstacles to fully utilizing these sophisticated time-dependent (hereditary) constitutive models in practical engineering analysis. These obstacles are 1) lack of efficient and robust integration algorithms and 2) difficulties associated with characterizing the large number of required material parameters, particularly when many of these parameters lack obvious or direct physical interpretations.

Generalized Viscoelastoplasticity with Potential Structure (GVIPS)

As most advanced material systems (for example metallic, polymer and ceramic-based systems) being currently researched and evaluated are for high temperature air frame and propulsion system applications, the required constitutive models must account for both **reversible** and **irreversible** time-dependent deformations. For example, considering that most aerospace engine designs are typically limited to the quasilinear stress and strain regimes, the reversible time-dependent response component becomes dominate in comparison to the irreversible component. Alternatively, one can envision another extreme case (e.g., in polymer and rubber based systems under varying temperatures) in which a purely reversible viscous response is present. And lastly, an obvious natural extension for general applicability is the middle ground in which a combined reversible and irreversible representation is required.

To this end, a coupled fully-associative viscoelastoplastic model has been formulated (Arnold & Saleeb, 1994; Saleeb et al., 2000), with sufficient generality in its potential functions to permit systematic introduction of multiple mechanisms for both viscoelastic (reversible) and viscoplastic (irreversible) response components (Fig. 3). The notions of strain and stress partitioning are introduced, leading to the additive decomposition of strain into reversible and irreversible parts, and the partitioning of the stress into: (i) its equilibrium (σ_e) and non-equilibrium ($q^{(n)}$) parts in the reversible region, and (ii) the internal ($\alpha^{(n)}$) and overstress ($\sigma - \alpha$) components in the irreversible region. The viscoelastic part utilizes the concept of equilibrium stress, leading to a rate dependency upon instantaneous loading, as well as to a unique limiting state of elastic defor-

mation at infinite times. The viscoplastic formulation accounts for both **nonlinear kinematic hardening** and **static recovery** sub-mechanisms. This general, multi-mechanism, hereditary deformation model has been shown to accurately represent a wide spectrum of material response under different loading conditions for the case of titanium alloys. Examples include 1) rate-dependent (effective) material tangent stiffness during initial loading or any subsequent reversed loading, 2) pure transient response (e.g., in creep or relaxation) within the reversibility region, 3) anelastic behavior upon stress reversal, irrespective of the load level, as well as, 4) the many response features that are common to 'unified viscoplastic' formulations already existing (e.g., rate-sensitivity, creep-plasticity interaction, thermal recovery etc.).

Armed with such an accurate and robust constitutive model one can utilize the correlated model as input to describe the various constituent (e.g., fiber and/or matrix) material behavior in a composite micromechanical deformation theory like the generalized method of cells (Aboudi, 1994) described in the following section. Alternatively, one can construct (using appropriate invariants) constitutive models beginning at the macroscale, wherein the composite is viewed as an anisotropic material in its own right, with its own experimentally measurable properties. Consequently, the material itself performs the homogenization procedure from the micro to the macroscale (see Fig. 1). Thus, as with polycrystalline monolithic alloys at elevated temperatures, the intrinsic, history dependent, interactive effects of the constituents (e.g. fiber, interface, and matrix) are embedded in the experimental results. Clearly, this theoretical approach lends itself to explicit experimental characterization and alleviates any assumptions, inherent to a micromechanical approach, concerning *in-situ* constituent response. Of course, the macromechanical approach is not universally applicable for the structural analysis of multiphased materials because its validity depends on characteristic structural dimensions, the severity of gradients (stress, temperature, etc.) in the structure, and the size (cell size) of the internal texture of the material (Aboudi et al., 1993; Onat and Wright, 1991).

Assuming this macro starting point, a number of anisotropic unified viscoplastic models at the macro (or composite) level have been proposed. Two such transversely isotropic viscoplastic models have been extended from their initially isotropic forms by the introduction of physically meaningful invariants (e.g., Robinson & Miti-Kavuma, 1994; Saleeb & Wilt 1993; Arnold et al., 1992; Robinson, 1987). The assumption of local transverse isotropy, by definition, limits the

strict applicability of these models to continuous reinforced composites with a single fiber orientation and a hexagonal fiber packing arrangement. Critical experiments in support of these extensions have been conducted on model ductile/ductile systems. The importance of prior history was illustrated through creep and creep-plasticity interaction experiments for both longitudinally (Arnold et al., 1992) and transversely (Arnold et al., 1993) reinforced specimens.

Integration Schemes

In early applications, the explicit integration schemes, (i.e., forward Euler method) were predominate because of their ease of implementation, and because they do not require evaluating and inverting a Jacobian matrix. However, with explicit integrators the solution may not be efficient, in that, too many load/time steps (see Fig. 4) may be required and convergence (stability) can not be guaranteed. Consequently, the majority of recent work has emphasized the use of implicit integration methods in view of their stability and convergence properties. The numerical integration scheme, adopted herein is the implicit **backward Euler** method (Saleeb & Wilt, 1993; Saleeb et al., 1998 and 2000) due to its unconditional **stability** and its **robustness**. A concise form has been developed by exploiting the mathematical structure of the model equations, lending to a very efficient implementation of the update and its **algorithmic** (consistent), (material) **tangent** stiffness. Furthermore, unique to the present model (compared to other state-variable representations) is the feature of complete potentiality or full **associativity** with the ensuing attributes of **symmetry** in all arrays involved in the implicit iterative scheme, including its algorithmic (consistent) **tangent** stiffness. Also, the **closed-form**, expressions for the tangent stiffness arrays are derived such that their dimensions are **independent** of the number of state variables employed (i.e., the stress tensor, tensorial viscoelastic internal parameters, and tensorial viscoplastic state variables). That is, the dimension is **only** determined by the underlying problem dimension (**six** for three-dimensional problems, **three** for plane stress problems, etc.) These expressions and the tangent stiffness have proved effective in implementing the Newton iterative scheme utilized in the integration and have been implemented, into the **ABAQUS** UMAT routine, in conjunction with the above described multimechanism **GVIPS** model. Figures 4 and 5 clearly illustrate, given a cyclic and nonproportional load path, respectively, the benefits of this approach, particularly in the context of large-scale FEA (Saleeb et al., 2000). Note that the explicit forward Euler scheme

completely failed during the nonproportional path (Fig. 5) even though thousands of steps per load segment were used.

Parameter Estimation

A key for the practical utility of the above mentioned viscoelastoplastic model is the development of a robust, stand-alone, Constitutive Material Parameter Estimator (**COMPARE**) for automatically characterizing the various time-dependent, nonlinear, material models. Efficient algorithms have been developed for the model's material parameter estimation, based on mathematical optimization techniques (see e.g., Vanderplaats, 1984); i.e., nonlinear least-square fitting (Saleeb et al. [1998]) under general stress / strain / mixed test controls (e.g., stress control in creep, mixed control under relaxation conditions, etc.), with time-variant response functionals. An essential ingredient here is the development of response sensitivity arrays, which have been shown to be directly linked to the algorithmic tangent stiffness arising from the integrated fields (stress and viscoelastic/viscoplastic internal state variables) in the update/time-stepping scheme utilized. The entire procedure is automated within a stand-alone computer software code (Saleeb et al., 1998) called **COMPARE** (Constitutive Material PARAmeter Estimator).

FATIGUE DAMAGE MODELING

Numerous approaches to modeling fatigue damage in a monolithic material have been proposed in the literature. However, the authors have selected to utilize Continuum Damage Mechanics (CDM) to describe the degradation of constituent materials. CDM is attractive because it allows one to describe the material's progressive deterioration (damage) from the virgin (or undamaged) state to that of the final state which corresponds generally to macrocrack initiation and propagation (or "breaking up") of the representative volume element of the material. The tracking or description of damage evolution is accomplished theoretically by the introduction of special thermodynamic (internal) field variables representing, in an appropriate statistical sense, the local distribution and density of defects.

Under cyclic loading (fatigue), the internal damage variable is associated with the initiation and propagation of transgranular defects (e.g., slip bands and micro-cracks) within a given constituent material. Here the isotropic fatigue CDM model proposed by Chaboche (1988a and

1988b) has been initially selected to establish the required numerical framework. This model: can i) can describe the evolution of a scalar measure of damage given a multiaxial state of stress, ii) has been demonstrated to be capable of predicting a wide range of constituent metallic materials, iii) can be incorporated into structural analysis codes through the appropriate user-definable routines, and iv) can be applied directly at either the micro- or macro-scale.

Assuming that the damage mechanisms discussed above on the microstructural scale of a constituent material occur on the mesoscale of the composite¹, extension of the previously mentioned isotropic fatigue damage model to the macrolevel can be accomplished. This extension is enabled through the introduction of anisotropic damage surfaces, such that transversely isotropic fatigue damage is predicted using the Anisotropic Damage Evolution And Life (ADEAL) model proposed by Arnold & Kruch (1991 and 1994). The anisotropy of these surfaces are defined through physically meaningful invariants which reflect the local stress states that are likely to influence strongly the various damage modes in metallic composites. Furthermore, although the damage is represented as a scalar (i.e., magnitude of damage is identical in all directions), the evolution (or accumulation) of damage is anisotropic and associated with the preferred direction of the material. Clearly, as in the case of deformation, such a macroscale approach lends itself to explicit experimental characterization and alleviates any assumptions, inherent in a micromechanical approach, regarding *in-situ* constituent degradation. This is an extremely attractive feature of the macro approach, since to date very little constituent degradation information is available in its "stand alone" form, and even less (if any) quantitative information is available in its "in-situ" state. Thus macroscale damage approaches can make full use of the extensive research conducted at the composite level.

MICROMECHANICS BASED ANALYSIS

A critical issue in the micromechanics-based analysis of composite structures becomes the availability of a computationally efficient homogenization technique (see Fig. 1) that is: 1)

¹For example, it is postulated that the surface or interface of a constituent (the fiber) plays a similar role on the mesostructural scale as the grain boundary of a constituent (grain) plays on the microscopic scale.

capable of handling the sophisticated, physically based, viscoelastoplastic constitutive and life models for each constituent, 2) able to generate accurate displacement and stress fields at both the macro and the micro levels and 3) compatible with the finite element method. The Generalized Method of Cells (GMC) developed by Paley and Aboudi (1992) is one such micromechanical model which has been shown to predict accurately the overall macro behavior of various types of composites given the required constituent properties. Specifically, the method provides "closed-form" expressions for the macroscopic composite response in terms of the properties, size, shape, distribution, and response of the individual constituents or phases that make up the material. Furthermore, expressions relating the internal stress and strain fields in the individual constituents in terms of the macroscopically applied stresses and strains are available through strain or stress concentration matrices. These expressions make possible the investigation of failure processes at the microscopic level at each step of an applied load history.

MAC/GMC (Arnold et al., 1999) enhances the basic capabilities of GMC by providing a modular framework wherein 1) various thermal, mechanical (stress or strain control) and thermomechanical load histories can be imposed, 2) different integration algorithms may be selected, 3) a variety of material constitutive models (both deformation and life) may be utilized and/or implemented, 4) a variety of fiber architectures (both unidirectional, laminate and woven) may be easily accessed through their corresponding representative volume elements contained within the supplied library of RVEs or input directly by the user, and 5) graphical post processing of the macro and/or micro field quantities is made available. Consequently, the availability of **MAC/GMC** (see, www.grc.nasa.gov/WWW/LPB/mac) now provides industry, academia and government engineers and materials scientists with a comprehensive, computationally efficient, user-friendly micromechanics analysis tool that can easily and accurately design/analyze multi-phase (composite) materials for a given application. **MAC/GMC** is also ideally suited for conducting sensitivity/parametric studies (i.e., "what-if" scenarios) in the design/analysis of advanced composite materials (e.g., MMCs, PMCs, and CMCs). Furthermore, **MAC/GMC** can be interfaced directly with standard linear and nonlinear finite element analysis packages (through their respective user definable constitutive routines) for cost-effective large-scale component design and analysis. Currently, such an interface exists only for HKS's nonlinear finite element

code, ABAQUS. For clarity this finite element implementation of MAC/GMC has been given its own unique name, FEAMAC.

To date over 35 industrial and academic customers have used or are using MAC/GMC for a variety of applications. In particular, FEAMAC is being employed by the Goodyear Tire and Rubber Co. and GRC to understand the influence of cord architecture on the behavior and performance of their tires, and by GRC and Boeing, Rocketdyne Division to design and analyze an MMC housing on a large 400-K thrust class turbopump. For illustration purposes, see Fig. 6, two 432 element (C3D8) idealizations of a 33 volume percent SCS-6/TIMETAL 21S test specimen, longitudinally and transversely reinforced, are analyzed. In Fig. 6a, a comparison of the macro response predication resulting from MAC/GMC and that coming from the center element within the gage length (where FEAMAC is providing the viscoplastic material response at all integration points throughout the specimen) is made. Clearly, the agreement is excellent. Furthermore in Fig. 6b, the macro von Mises stress contours for both specimens and the corresponding in-situ micro stress and inelastic strain field within each constituent are illustrated at the end of the applied tension test. Note that in the transverse specimen fiber-matrix debonding has been enabled denoted by the diamond shaped interface in Fig. 6b.

COMBINED DEFORMATION/DAMAGE

Historically, in predicting the fatigue lives of structures there are basically two approaches used: uncoupled or fully coupled deformation-damage methods. In the traditional uncoupled analysis, the damage due to fatigue is assumed not to effect the deformation of the structure, whereas in a coupled analysis, the evolution of material damage is integrated (coupled) with the incremental finite element analysis (by utilizing the concept of effective stress) so that as the analysis progresses and damage propagates, stress redistribution occurs throughout the structure during subsequent load cycles. Recently, a coupled/uncoupled deformation and damage algorithm (Wilt & Arnold, 1994) utilizing the multiaxial, isothermal, continuum based fatigue damage model ADEAL for unidirectional MMCs (discussed earlier) has been implemented into the commercial finite element analysis codes, MARC (see Wilt et al., 1993) and ABAQUS, as well as MAC/GMC (see Arnold et al., 1999). This coupled deformation and damage algorithm

has been applied on both the micro and macro scales, wherein the microscale application utilizes the respective isotropic simplifications of the various anisotropic damage models.

The application on the micro scale consisted of analyzing a SiC/Ti-15-3 composite employing a unit cell with a square pack arrangement and a 35 percent volume fraction of fibers (Wilt et al., 1997). Alternatively, the macroscale application involved the analysis and experimental characterization (Gravett and deLanauville, 1993) of a SiC/Ti-15-3 MMC ring insert consisting of a composite core and matrix cladding (Arnold and Wilt, 1993; Wilt et al., 1997). The resulting design life curves for both a coupled and uncoupled analysis are shown in Fig. 7. Note how the uncoupled curves only simulates initiation of damage at a given location, e.g. ID or OD, where the coupled analysis predicates failure of the ring structure, as it includes both initiation and propagation of damage. Also, the corresponding damage profiles for the coupled analysis are shown at 20% and 100% of the life of the structure. Note that at 20% of life, damage has initiated at the inner boundary of the composite core.

The above two applications serve to demonstrate the applicability of the fatigue damage model and the associated algorithm to both macro (structural) and micromechanical analyses. Also as an aside, the above algorithm can be extended easily to incorporate creep-fatigue interaction effects both on the micro and macro scales (Arnold & Kruch, 1991 and Kruch & Arnold, 1997).

ACKNOWLEDGEMENTS

Second, third and fourth authors would like to acknowledge the financial support provided by NASA Glenn Research Center under grants (NAG3-1747 and NCC3-441) to the University of Akron

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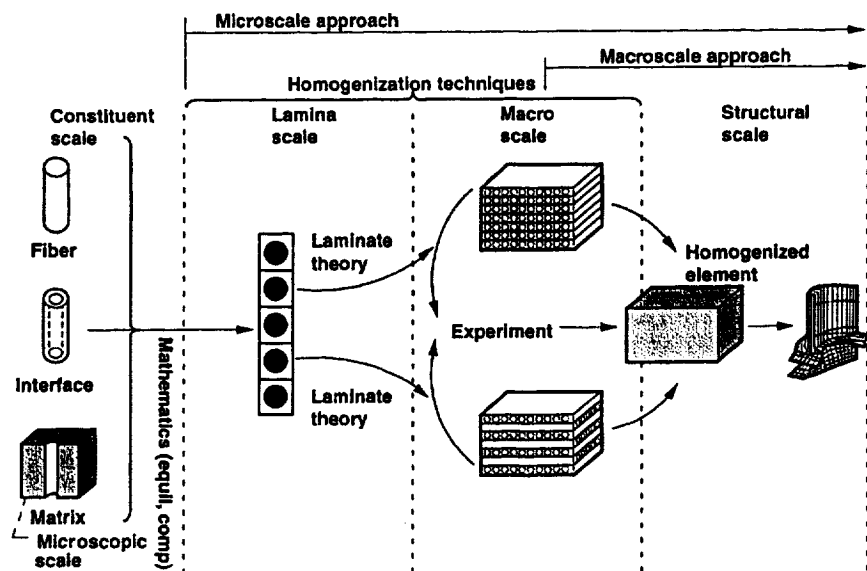


Figure 1 Illustration of levels of scale and approaches for composite analysis

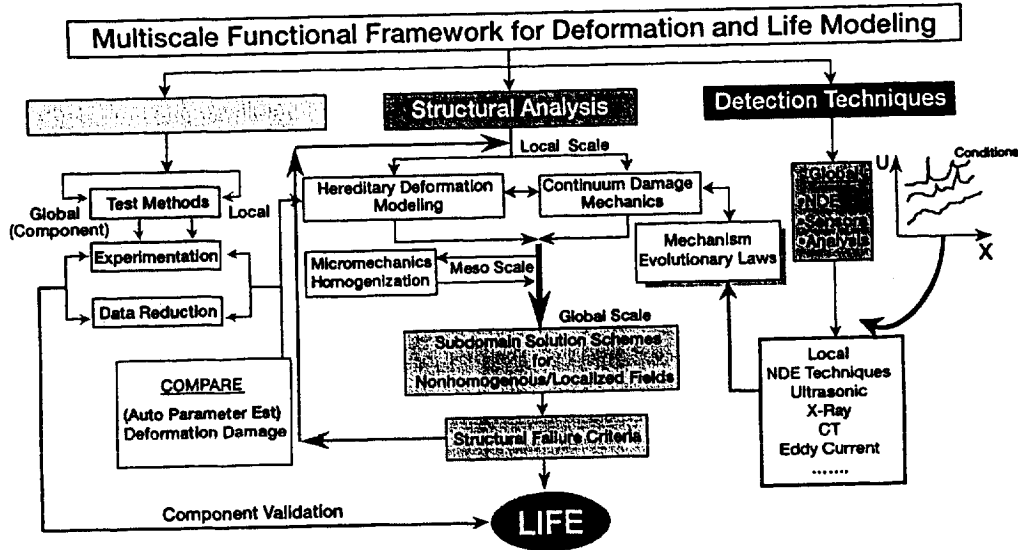


Figure 2 Schematic describing Multiscale Functional Framework for Deformation and Life Modeling

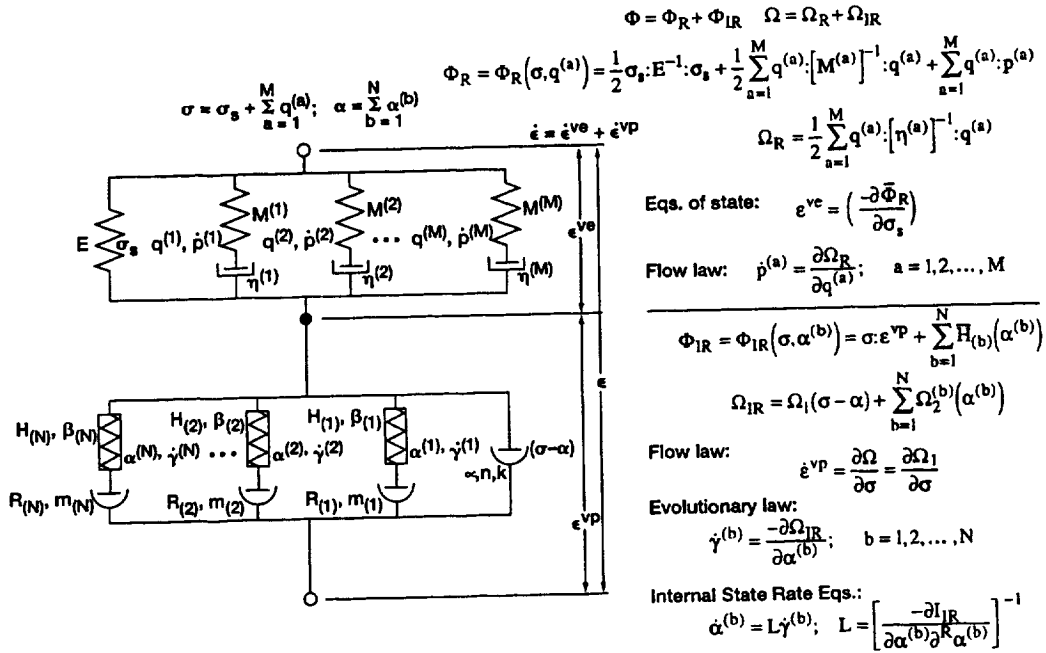


Figure 3 Summary of the stress and strain partitioning of the General Multimechanism Hereditary behavior model.

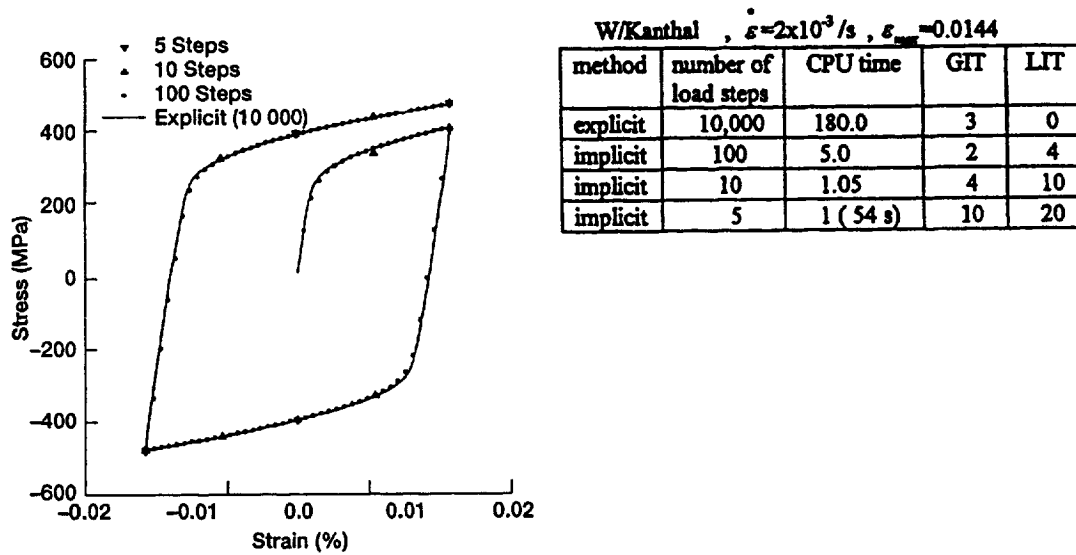


Figure 4 Results illustrating the efficiency of the numerical implementation of GVIPS under cyclic conditions

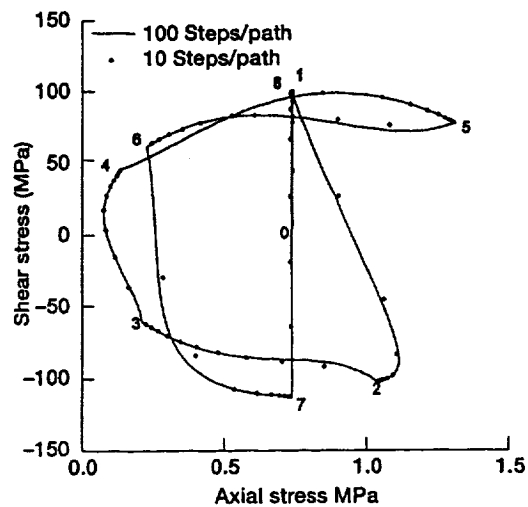


Figure 5 Results illustrating the efficiency of the numerical implementation of GVIPS under nonproportional loading conditions

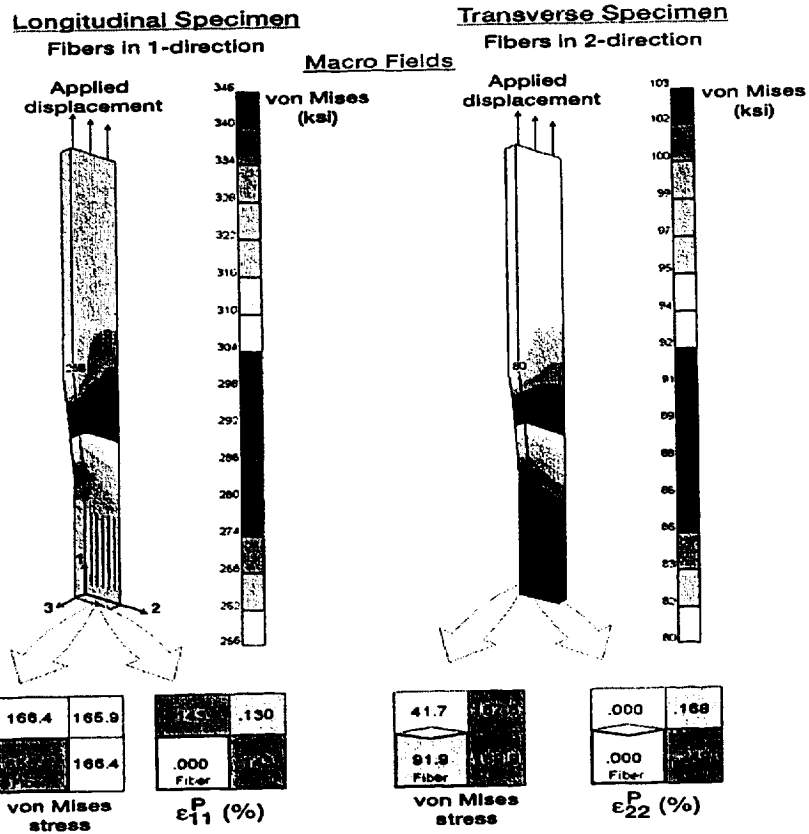
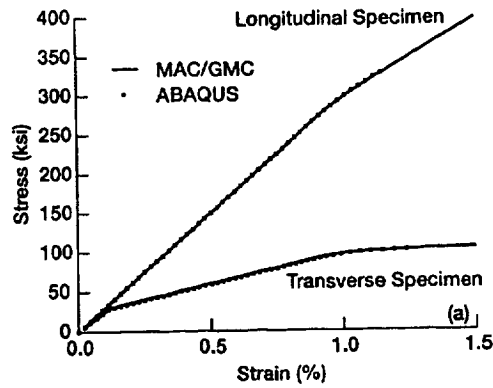


Figure 6 Micromechanics-based structural analysis results of both longitudinally and transversely reinforced SCS-6/TIMETAL 21S dogbone test specimens. a) Macrolevel stress-strain response. b) Multilevel ABAQUS results using FEAMAC to represent material behavior.

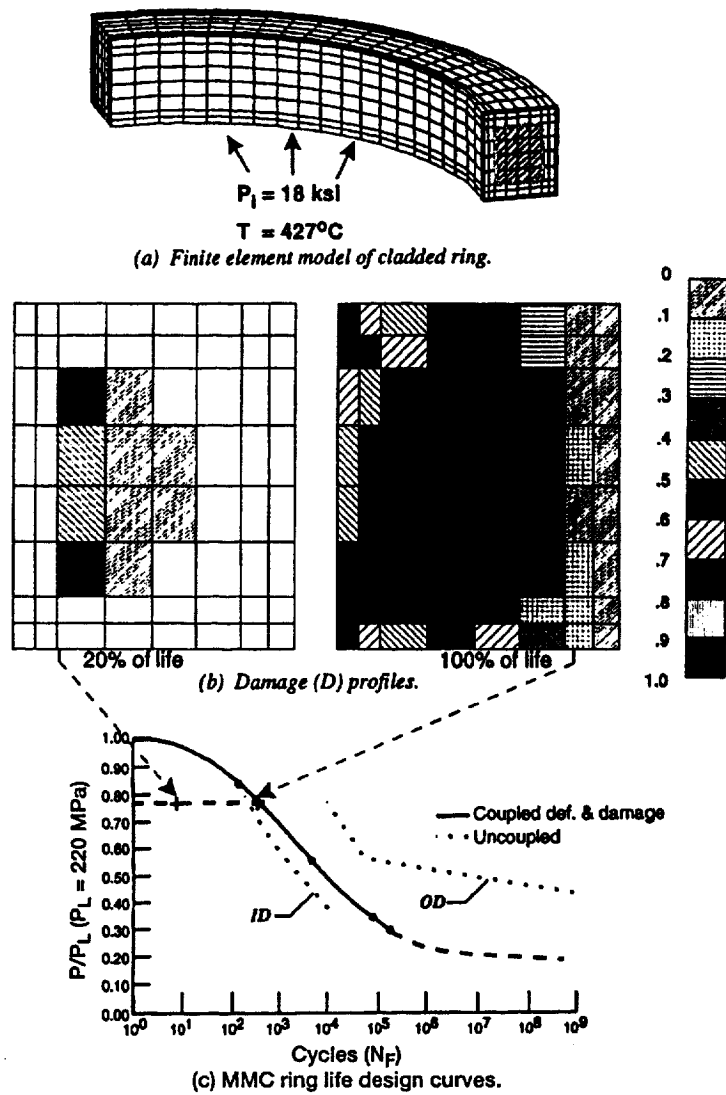


Figure 7 Prediction of fatigue life and damage evolution in a TMC ring insert a) Finite element model of cladded ring. b) Damage (D) profiles and c) MMC ring life design curves.